Lecture 1:
Introduction to Course, Postulates of QM, and Vector Spaces

Date Revised: 2008/09/29
Date Given: 2008/09/29

Section 1
Introduction to Course

Course Logistics

- The course webpage is

  http://www.astro.caltech.edu/~golwala/ph125ab/

  Much of the material will be linked from the course Moodle page, which you can access from the above page or directly via

  https://courses.caltech.edu

  A password for the Ph125a page will be provided in class; you can also obtain it from your classmates, the TAs, or myself. All course logistics and assignments will be announced via the Moodle page. You will find a listing of the course syllabus, problem sets, and solutions there. There is also a weekly homework survey. It would be very beneficial (to me and you) if you could fill out the survey regularly. Especially important is the "News Forum", via which I will make course announcements that I believe you will receive automatically via email once you have logged in to the course page. This is the first time Moodle is in widespread use at Caltech, and the first time I am using it, so please bear with me as I figure it out.

  Comments on the course (or the Moodle page) via the Moodle website are welcome and encouraged. Unfortunately, such comments are not anonymous, so please use campus mail to one of my mailboxes if anonymity is desired.
- Text: Shankar, lecture notes. Many other nice texts are available, choose a different one if you don't like Shankar. See the course reserve list.
- Syllabus: Detailed syllabus on web. Stay on top of it!

Course Logistics (cont.)

- Problem sets: one per week, 4-6 problems. Posted via web site. Due date: **Tuesday, 4 pm**. Problem sets will be much easier to complete in a reasonable amount of time if you stay on top of lectures and clarify any confusion on material *before* you begin the problem set. Solutions posted on web shortly after set is due, graded sets handed back by end of following week. Keep a copy of your problem sets if you want to check your work against the solutions promptly (waiting 1.5 weeks is a bad idea...).
- Grading: 1/3 problem sets (weekly), 1/3 midterm, 1/3 final. (No problem set during week that midterm is due.)
- Exams: each will be 4 hours, 4-6 problems, take home, 1 week lead time. Should only take 2 hours.
- Class attendance: not mandatory. If you don't find it useful, then don't come. The lecture notes will be posted online promptly. But please make the decision based on a careful evaluation of whether you find lecture useful, not on your sleep schedule or time pressure from other classes. And, most importantly, do not think that, just because all the course material is available online, you can catch up the night before the problem set or exam is due and do well. If you don't attend class, be disciplined about doing the reading and following the lecture notes.
- Office hours: I will hold an evening office hour the night before problem sets are due. I strongly prefer Monday night 7-9 pm. There will be a TA office hour also.
- TAs will be primarily responsible for solution sets and grading. They will rotate through the TA office hour.

Course Material

In this course, you will learn to attack basic quantum mechanical problems from scratch and arrive at full solutions that can be tested by experiment. You will see much material that is familiar to you from Ph2/12, but we will cover that material more deeply and with a more formal foundation that will provide you the tools to attack new problems, whether in other courses or in research.

Course Material (cont.)

Prerequisites

Physics:

- Quantum mechanics: None required, in principle. While most students taking this course will have had a course in quantum mechanics before at the level of Ph 2/12, we develop all concepts from scratch and do not require that you recall results from a previous course. However, because we take a formal, systematic approach, basic familiarity with quantum mechanics at the level of Ph 2/12 will be helpful in motivating various parts of the course — essentially, in seeing where we are going. *If you have never had a QM course before at the level of Ph 2/12, you will have to judge for yourself whether you are ready for this course or not.*
- Classical mechanics: Nothing more than Ph1a-level classical mechanics is required. Where we need more sophisticated concepts, we will provide the necessary background material. Knowledge of Hamiltonian mechanics will help in motivating some of the concepts we deal with, but is not necessary and will not be assumed.

Course Material (cont.)

Mathematics:

- Multivariate differential and integral calculus in cartesian and non-cartesian (cylindrical and spherical) coordinate systems at the level of Ph1abc.
- Vectors and vector operations at the level of Ph1abc.
- Methods for solving first- and second-order linear ordinary differential equations at the level of Ph1abc (exponentials and simple harmonic oscillators).
- We will use separation of variables to solve first- and second-order linear partial differential equations, but we will not assume you already know how.
- Linear algebra: We do not assume any prior knowledge of linear algebra aside from matrix multiplication and systems of linear equations (essentially, high-school algebra) along with glancing familiarity with concepts like orthogonal and symmetric matrices. We will develop the necessary more sophisticated concepts here. However, you must quickly become adept in linear algebra because it is the *language* of quantum mechanics. Linear algebra must become second nature to you.
- Key point: Mathematics is the language of physics. You must be competent in above basic mathematical physics in order to understand the material in this course. Intuition is important, but few can succeed in physics without learning to formalize that intuition into mathematical concepts and calculate with it.

Course Material (cont.)

Topics to be covered:

- Mathematical foundations for QM.
- Fundamental postulates of QM: our framework for how we discuss states, physical observables, and interpret quantum states.
- Simple one-dimension problems — building your intuition with piecewise-constant potentials.
- Harmonic Oscillator — the archetypal QM problem.
- Commutations and uncertainty relations — how the noncommutativity of the operators for physical observables results in minimum uncertainties when performing noncommuting measurements.
- Multiparticle systems: Fock product spaces, treatment of systems of identical particles (symmetry/antisymmetry of states).
- Approximate methods for problems without exact solutions: WKB approximation, variational method.
- Classical rotations in three spatial dimensions; tensors.
- Symmetries: esp. how symmetries of the Hamiltonian determine conserved observables.
- Coordinate angular momentum. How to use the angular momentum observables to classify 3D states.

Course Material (cont.)

- Formalism for spin angular momentum.
- Addition of angular momentum: how to decompose a product of two different angular momenta into a set of single system angular momenta.
- Time-independent perturbation theory: How to approach problems in which the Hamiltonian contains small noncommuting terms.
- Hydrogen atom, including perturbations.
- Connections to classical mechanics: classical limits, symmetries, Hamiltonian formalism, Hamilton-Jacobi equation.

Section 2
Postulates of Quantum Mechanics

Summary

1. The state of a particle is represented by a vector in a Hilbert space.
2. The fundamental state variables x and p of classical mechanics are replaced by Hermitian operators X and P whose matrix elements are well specified in a Hilbert space basis consisting of position eigenstates (states with perfectly defined position x). Any derived dynamical variables $\omega(x, p)$ are replaced by operators Ω defined by the above correspondence.
3. Measurement of any classical variable $\omega(x, p)$ for a quantum state yields only the eigenvalues of the corresponding operator Ω, with the probability of obtaining the eigenvalue ω given by the squared norm of the projection of the state onto the eigenstate corresponding to ω.
4. The state vector evolves according to the Schrödinger equation.

Postulate 1: Representation of Particle States

The state of a particle is represented by a vector $|\psi(t)\rangle$ in a Hilbert space.

What do we mean by this?

We shall define Hilbert space and vectors therein rigorously later; it suffices to say for now that a vector in a Hilbert space is a far more complicated thing than the two numbers x and p that would define the classical state of a particle; the vector is an infinite set of numbers.

The only useful immediate inference we can draw from this statement on its own, based on the definition of *Hilbert space* and *vector*, is that states can be combined linearly. This is interesting, as there is no classical analogue to linear combination of states; for example, if a classical particle only has access to classical state 1 with phase space coordinates (x_1, p_1) and classical state 2 with (x_2, p_2), the particle can only be in one or the other; there is no way to "combine" the two states. Another way of saying this is that quantum mechanics provides for "superposition" of states in a way that classical mechanics does not. But, while interesting, it is not clear what this means or what the experimental implications might be.

Postulate 1: Representation of Particle States (cont.)

The state of a particle is represented by a vector $|\psi(t)\rangle$ in a Hilbert space.

We will see below that Postulates 1 and 3 give rise to the interpretation of the state vector as an object that gives the probability of measuring a particular value for a particular classical observable, depending on what Hilbert space basis the vector is written in terms of. Typically, $|\psi\rangle$ is written in terms of the position basis (a set of Hilbert space vectors with well-defined particle position), in which case $|\psi\rangle$ will give the probability of finding the particle at a given position.

Postulate 2: Correspondence for Classical Variables

The independent variables x and p that describe completely the state of a particle in classical mechanics are represented by Hermitian operators X and P in the Hilbert space of states, with X and P having the following matrix elements when using the position basis for the Hilbert space:

$$\langle x\,|X\,|x'\,\rangle = x\delta\left(x-x'\right) \qquad \langle x\,|P\,|x'\,\rangle = -i\,\hbar\,\frac{d}{dx}\delta\left(x-x'\right) \tag{2.1}$$

We know x and p completely define the classical state of a particle because Newton's Second Law is a second-order differential equation: once x and its first derivative (via p) are specified at an instant in time, all higher-order derivatives are specified.

Postulate 2: Correspondence for Classical Variables (cont.)

The independent variables x and p that describe completely the state of a particle in classical mechanics are represented by Hermitian operators X and P in the Hilbert space of states, with X and P having the following matrix elements when using the position basis for the Hilbert space:

$$\langle x\,|X|x'\,\rangle = x\delta\left(x-x'\right) \qquad \langle x\,|P|x'\,\rangle = -i\,\hbar\,\frac{d}{dx}\delta\left(x-x'\right) \tag{2.2}$$

That is: Pick a basis for the Hilbert space of states that consists of position eigenstates, states that have definite, perfectly defined position. These of course may not be eigenstates of the Hamiltonian and thus may not have definite energy, but we don't care; we don't know about the Hamiltonian yet or the intepretation of its eigenstates. Then, everywhere we see in classical mechanics the position variable x, we replace it with the operator X whose matrix elements are defined as above for any pair of position basis states. This statement is almost a tautology: pick position basis states; then define the X operator such that the position basis states $\{|x\,\rangle\}$ are orthogonal eigenstates of the X operator with eigenvalues $\{x\delta(0)\}$.[a]

[a] We will define and discuss in detail δ functions later.

Postulate 2: Correspondence for Classical Variables (cont.)

The independent variables x and p that describe completely the state of a particle in classical mechanics are represented by Hermitian operators X and P in the Hilbert space of states, with X and P having the following matrix elements when using the position basis for the Hilbert space:

$$\langle x\,|X|x'\,\rangle = x\delta\left(x-x'\right) \qquad \langle x\,|P|x'\,\rangle = -i\,\hbar\,\frac{d}{dx}\delta\left(x-x'\right) \tag{2.3}$$

Why operators? Why are the operators fully specified by matrix elements? Why Hermitian?

We posit that classical variables are replaced by operators because, given the Hilbert space of particle states, the only way to extract real numbers corresponding to classical variables is to assume that there are operators that map from the Hilbert space to itself; such operators are completely specified by their matrix elements between pairs of states in the Hilbert space, and those matrix elements provide the necessary numbers. Why the operators must be Hermitian will be seen in Postulate 3.

Why can we not posit a simpler correspondence, that the operators X and P simply map from the Hilbert space to the real numbers? Because such a framework would just be classical mechanics, for we would be able to assign a specific value of x and p to each state $|\psi\,\rangle$ via $x = X\,|\psi\,\rangle$ and $p = P\,|\psi\,\rangle$.

Postulate 2: Correspondence for Classical Variables (cont.)

Any arbitrary classical dynamical variable $\omega(x, p)$ has a corresponding Hermitian operator

$$\Omega(X, P) = \omega(x \to X, p \to P) \tag{2.4}$$

where we simply replace x and p in ω with X and P to obtain $\Omega(X, P)$.

This is a fairly obvious extension of the first part of this postulate. It is predicated on the fact that any classical variable ω must be a function of x and p because x and p completely define the classical particle state. Since we have above specified a correspondence rule for x and p, this statement carries that rule through to all classical variables.[a]

[a] We shall consider later the complication that arises when ω includes products of x and p; because X and P are non-commuting operators, some thought must be put into how to order X and P in the correspondence.

Postulate 3: Results of Measurements of Classical Variables

Let $\{|\omega\rangle\}$ denote the set of eigenstates of the Hermitian operator with eigenvalues ω. If a particle is in an arbitrary state $|\psi\rangle$, then measurement of the variable corresponding to the operator Ω will yield only the eigenvalues $\{\omega\}$ of Ω. The measurement will yield the particular value ω for that variable with relative probability $P(\omega) = |\langle\omega|\psi\rangle|^2$ and the system will change from state $|\psi\rangle$ to state $|\omega\rangle$ as a result of the measurement being made.

This postulate puts physical meaning to postulates 1 and 2. Those postulates say how we define the particle state and what we replace our classical variables with. This postulate tells us how those operators extract information from the states.

This postulate hinges on the mathematical statement that any valid physical variable operator Ω has eigenstates with eigenvalues. This is just a mathematical result of the assumptions that the states live in a Hilbert space and that the operators Ω must be Hermitian.

At a conceptual level, the postulate means that measurement of a physical quantity *is* the action of the corresponding operator on the state.

Postulate 3: Results of Measurements of Classical Variables (cont.)

Let $\{|\omega\rangle\}$ denote the set of eigenstates of the Hermitian operator with eigenvalues ω. If a particle is in an arbitrary state $|\psi\rangle$, then measurement of the variable corresponding to the operator Ω will yield only the eigenvalues $\{\omega\}$ of Ω. The measurement will yield the particular value ω for that variable with relative probability $P(\omega) = |\langle\omega|\psi\rangle|^2$ and the system will change from state $|\psi\rangle$ to state $|\omega\rangle$ as a result of the measurement being made.

But let's break the statement down carefully:

1. The eigenvalues of Ω are the only values the measured quantity may take on.
2. The measurement outcome is fundamentally probabilistic, and the relative probability[a] of a particular allowed outcome ω is given by finding the projection of $|\psi\rangle$ onto the corresponding eigenstate $|\omega\rangle$. This of course implies that, if $|\psi\rangle$ is an eigenstate of Ω, then the measurement will always yield the corresponding eigenvalue.
3. The measurement process itself changes the state of the particle to the eigenstate $|\omega\rangle$ corresponding to the measurement outcome ω.

---

[a] By *relative* probability, we simply mean that the ratio of the probabilities of two outcomes is given by $P(\omega_1)/P(\omega_2) = |\langle\omega_1|\psi\rangle|^2 \,/\, |\langle\omega_2|\psi\rangle|^2$. The *absolute* probability of a particular outcome requires a normalizing factor that sums over all possible measurement outcomes, to be discussed later.

Postulate 3: Results of Measurements of Classical Variables (cont.)

Let $\{|\omega\rangle\}$ denote the set of eigenstates of the Hermitian operator with eigenvalues ω. If a particle is in an arbitrary state $|\psi\rangle$, then measurement of the variable corresponding to the operator Ω will yield only the eigenvalues $\{\omega\}$ of Ω. The measurement will yield the particular value ω for that variable with relative probability $P(\omega) = |\langle\omega|\psi\rangle|^2$ and the system will change from state $|\psi\rangle$ to state $|\omega\rangle$ as a result of the measurement being made.

The above points are far more than mathematics: they make assumptions about the relationship between physical measurements and the mathematical concepts of eigenstates and eigenvectors.

One could have assumed something simpler: that the measurement outcome is not probabilistic, but is rather the weighted mean of the eigenvalues with $|\langle\omega|\psi\rangle|^2$ providing the weighting factors; and that the act of measurement does not change $|\psi\rangle$. But this would be very similar to classical mechanics.

The assumptions we have chosen to make are the physical content of quantum mechanics and are what distinguish it from classical mechanics.

Postulate 4: Time Evolution of States

The time evolution of the state vector $|\psi(t)\rangle$ is governed by the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle \tag{2.5}$$

where $H(X, P)$ is the operator obtained from the classical Hamiltonian $\mathcal{H}(x, p)$ via the correspondence $x \longrightarrow X$ and $p \longrightarrow P$.

This statement requires little motivation at a general level: clearly, there must be some time evolution of $|\psi\rangle$ in order for there to be any interesting physics.

There is of course the technical question: why this particular form? One can, to some extent, derive the Schrödinger Equation in various ways, but those methods rely on assumptions, too.[a] Those assumptions may be more intellectually satisfying than simply postulating the Schrödinger Equation, but they provide no definite proof because they simply rely on different assumptions. Experiment provides the ultimate proof that this form is valid.

[a] We shall discuss some of these derivations later when we connect quantum mechanics to classical mechanics at a technical level.